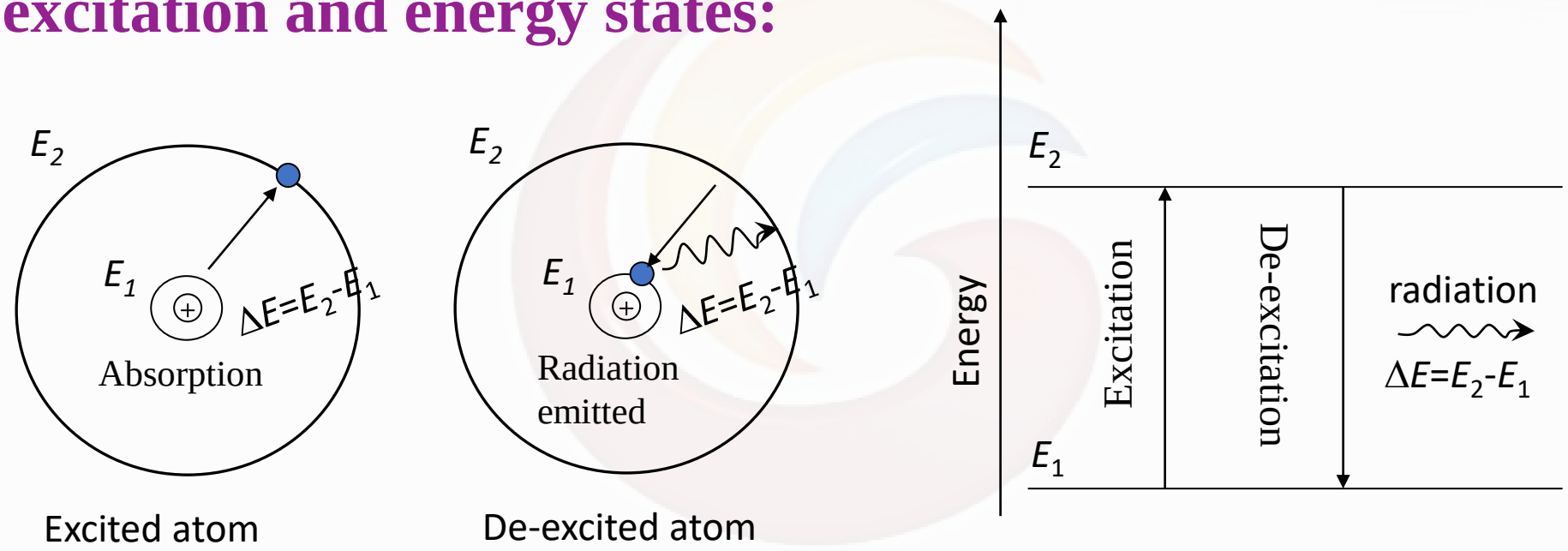
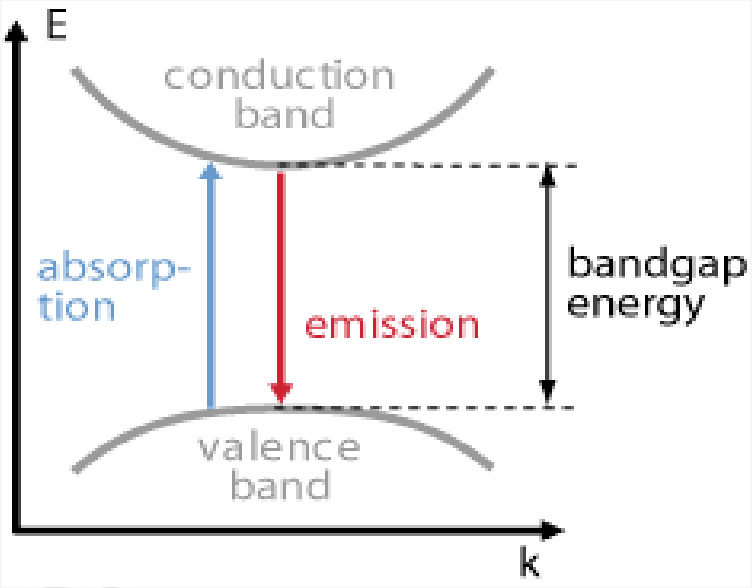
Atomic excitation and energy states:



According to the fundamentals of atomic structure, we know that in an atom, an electron in a ground state is stable and moves continuously in its orbit without radiating energy. When the electron receive an amount of energy equal to the difference of the energy of the ground state and one of the excited states (ΔE=E2-E1), it absorbs energy and jumps to excited states. The electron can stay very short time (lifetime ~10^{-8} s) in the excited state, but sometime may stay in the metastable state having relatively longer lifetime (~10-3 s). Note that an excited atom, while de-exciting, is not required to return to same state where it got excited. When this excited electron comes to the ground stete by the process of de-excitation, then it releases a radiation of energy ΔE=E2-E1. see the figure above.

Concept in Optical Transitions in Bulk Semiconductors

In semiconductors electrons can make transitions between two energy states and create or destroy photons in the process. In particular, transitions between the conduction band and the valence band ('inter band transitions') are optically active, as the lower conduction band generally consists of s-like states while the upper valence band consists of p-like states. Spontaneous emission, absorption, and stimulated emission can all take place between conduction band states and valence band states.

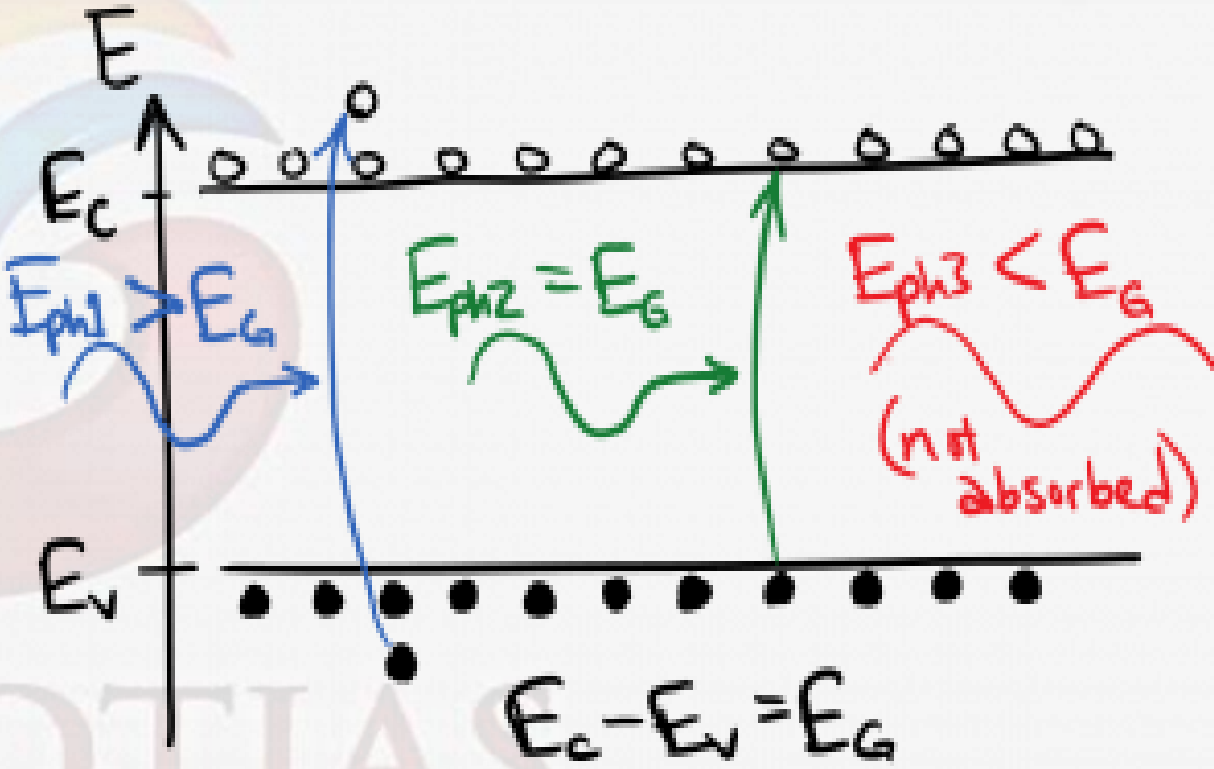


Concept in Optical Transitions in Bulk Semiconductors

Let's consider absorption first. As before, the ingredients for optical absorption are an incoming photon, a valence band energy state occupied by an electron, and an empty conduction band energy state. In equilibrium, the valence band is mostly full and the conduction band is mostly empty, so these conditions are easily met. Recall that optical absorption between two states in an atom only occurred for a narrow spectrum of photon energies (the linewidth of the transition). By contrast, optical absorption in a semiconductor can occur over a wide range of photon energies, as long as the photon energy is greater than or equal to the band gap energy.

Concept in Optical Transitions in Bulk Semiconductors

Since the absorption process creates an electron in the conduction band and a hole in the valence band, it is also called optical generation. Note that electrons created at energies higher than the band edge will quickly relax to the lowest conduction band energy states (band edge states) by releasing phonons. Similarly, holes created deep in the valence band will 'float up' to the valence band edge.



Concept in Optical Transitions in Bulk Semiconductors

Moving on to spontaneous emission, this process requires a conduction band energy state occupied by an electron and an empty valence band energy state (we can shorten this to say 'requires an electron and a hole', since 'electron' generally refers to an electron in the conduction band). This is the opposite of the common situation in equilibrium, but at a finite temperature there will be a small number of full states in the conduction band and empty states in the valence band.

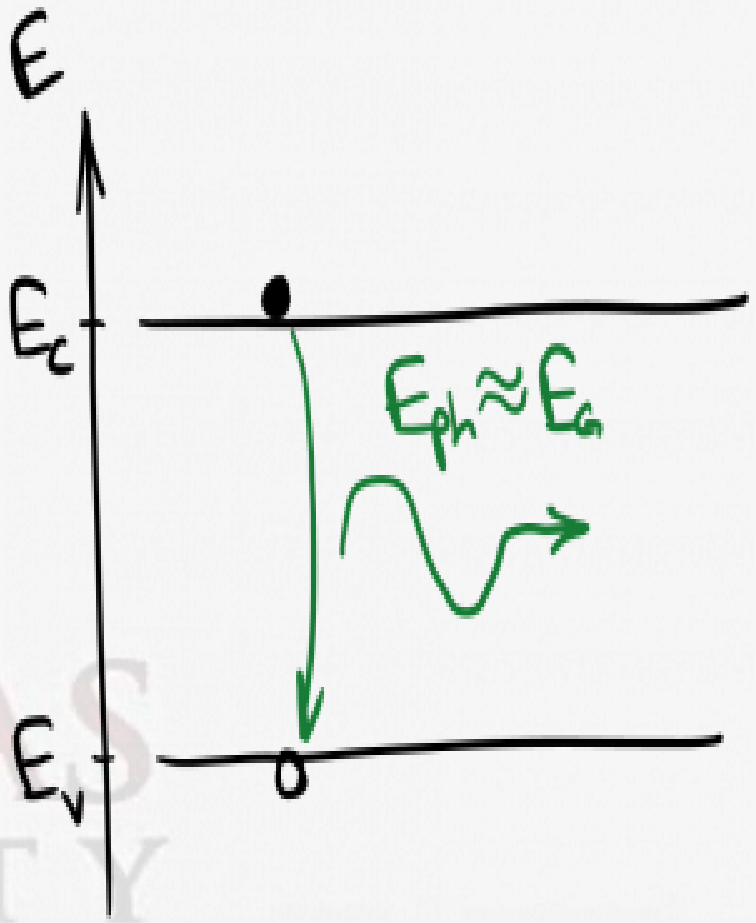
Concept in Optical Transitions in Bulk Semiconductors

Also, electrons and holes can be created via optical absorption and other pumping mechanisms we'll describe later. As with absorption, the spontaneous emission process is possible for a wide range of photon energies above the band gap; but in practice, the conduction band states most likely to be full are those lowest in energy, just as the valence band states most likely to be empty are those highest in energy. Therefore, the spontaneous emission observed from a semiconductor sample is most likely to have a photon energy nearly equal to the band gap energy. This is diagrammed below.

Concept in Optical Transitions in Bulk Semiconductors

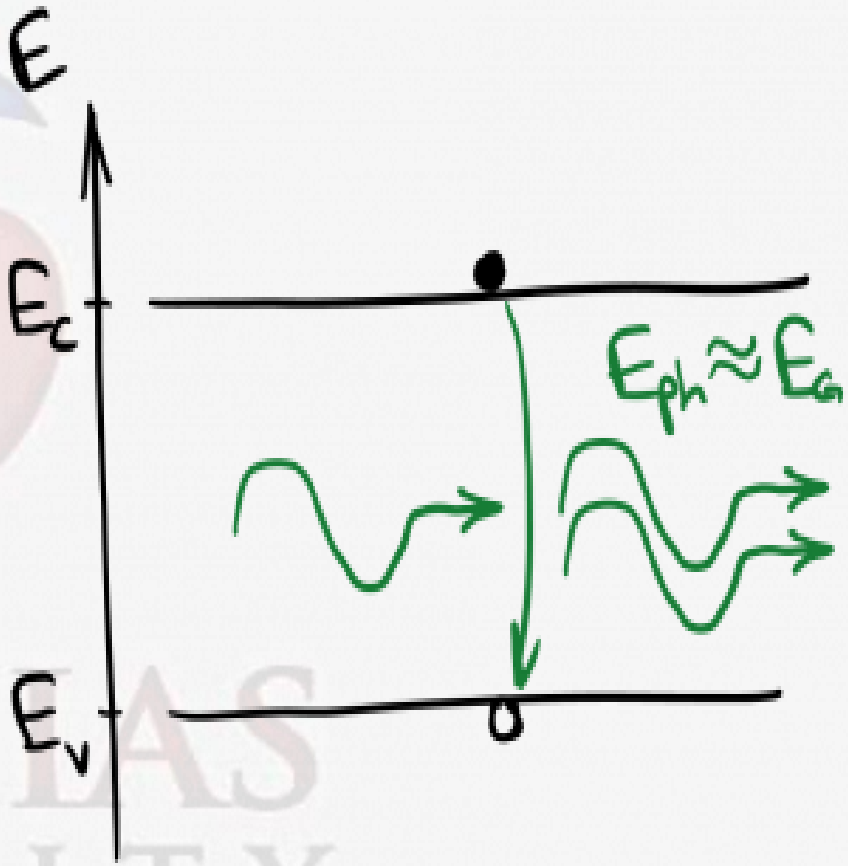
Since the spontaneous emission process 'destroys' an electron and a hole, it is also called spontaneous optical recombination.

At this point we can understand why ordinary silicon is not useful for light emission. As we saw, silicon has an indirect bandgap. That means that the lowest energy states in the conduction band have a different momentum than the highest energy states in the valence band. Unfortunately, those are the states that are most likely to be occupied by an electron and a hole, respectively. The spontaneous emission process must conserve both energy and momentum, but photons carry very little momentum (not zero!). Therefore, an electron at the 'bottom' of the conduction band is unable to recombine with a hole at the 'top' of the valence band via spontaneous photon emission, because that would violate conservation of momentum: the electron would have to undergo a significant momentum change, and the photon is unable to carry away enough momentum. The same logic also prevents stimulated emission in indirect band gap semiconductors.



Concept in Optical Transitions in Bulk Semiconductors

Finally we have stimulated emission, the most important process for laser operation. As before, this process requires an incoming photon, an electron, and a hole. It produces a copy of the incoming photon. As with spontaneous emission, we expect that in most cases the stimulated emission will occur primarily between band-edge states, as these states are most likely to be occupied with electrons and holes. Thus, semiconductor optical amplifiers generally amplify light whose photon energy is approximately equal to the band gap energy of the semiconductor gain medium. The stimulated emission process is diagrammed below.



Concept in Optical Transitions in Bulk Semiconductors

Since the stimulated emission process ‘destroys’ an electron and a hole, it is also called stimulated optical recombination. In order to make stimulated emission the dominant optical process, we need to achieve population inversion.

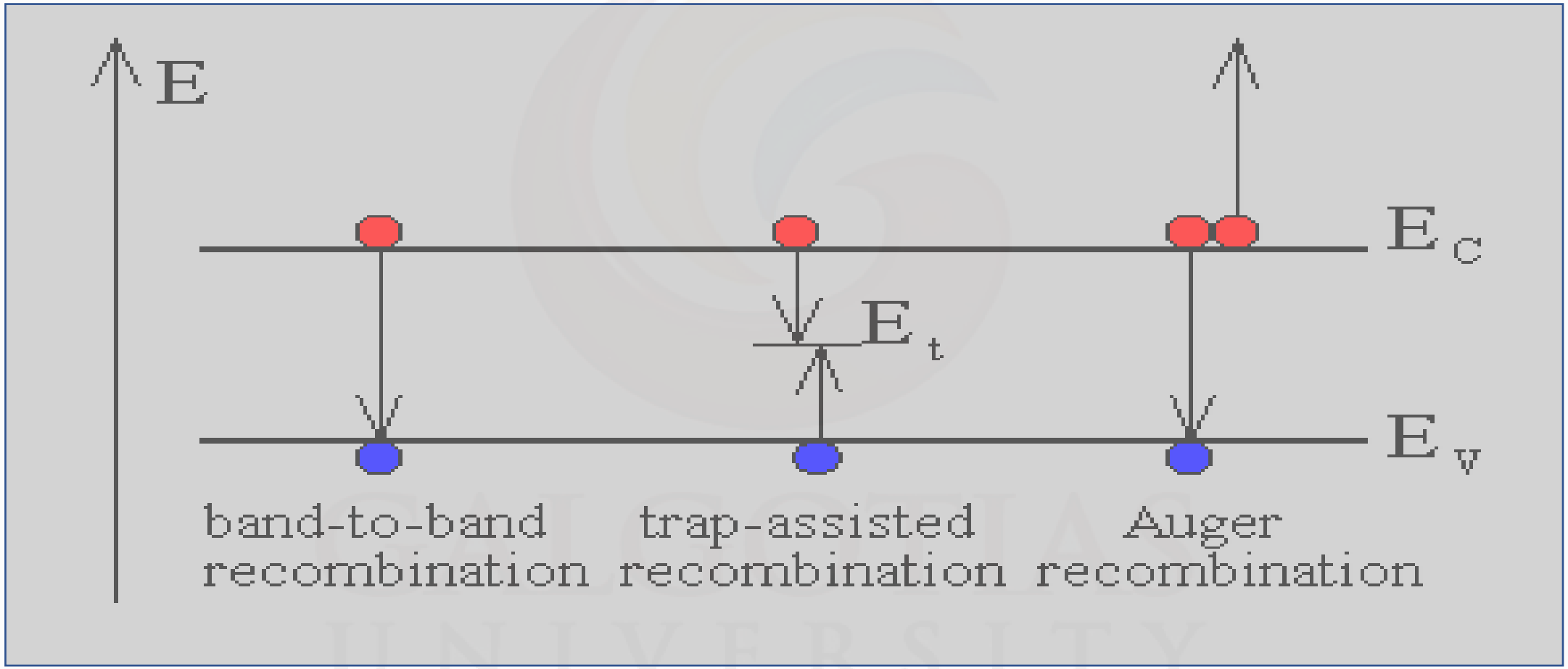
Recombination Process

- Recombination of electrons and holes is a process by which both carriers annihilate each other: the electrons fall in one or multiple steps into the empty state which is associated with the hole. Both carriers eventually disappear in the process.

- The energy difference between the initial and final state of the electron is given off. This leads to one possible classification of the recombination processes: In the case of radiative recombination this energy is emitted in the form of a photon, in the case of non-radiative recombination it is passed on to one or more phonons and in Auger recombination it is given off in the form of kinetic energy to another electron.

- Another classification scheme considers the individual energy levels and particles involved. These different processes are further illustrated with the figure below.

Recombination Process



Carrier recombination mechanisms in semiconductors

Recombination Process

Band-to-band recombination occurs when an electron falls from its state in the conduction band into the empty state in the valence band which is associated with the hole. This band-to-band transition is typically also a radiative transition in direct bandgap semiconductors.

Trap-assisted recombination occurs when an electron falls into a "trap", an energy level within the bandgap caused by the presence of a foreign atom or a structural defect. Once the trap is filled it can not accept another electron. The electron occupying the trap energy can in a second step fall into an empty state in the valence band, thereby completing the recombination process. One can envision this process either as a two-step transition of an electron from the conduction band to the valence band or also as the annihilation of the electron and hole which meet each other in the trap. We will refer to this process as Shockley-Read-Hall (SRH) recombination.

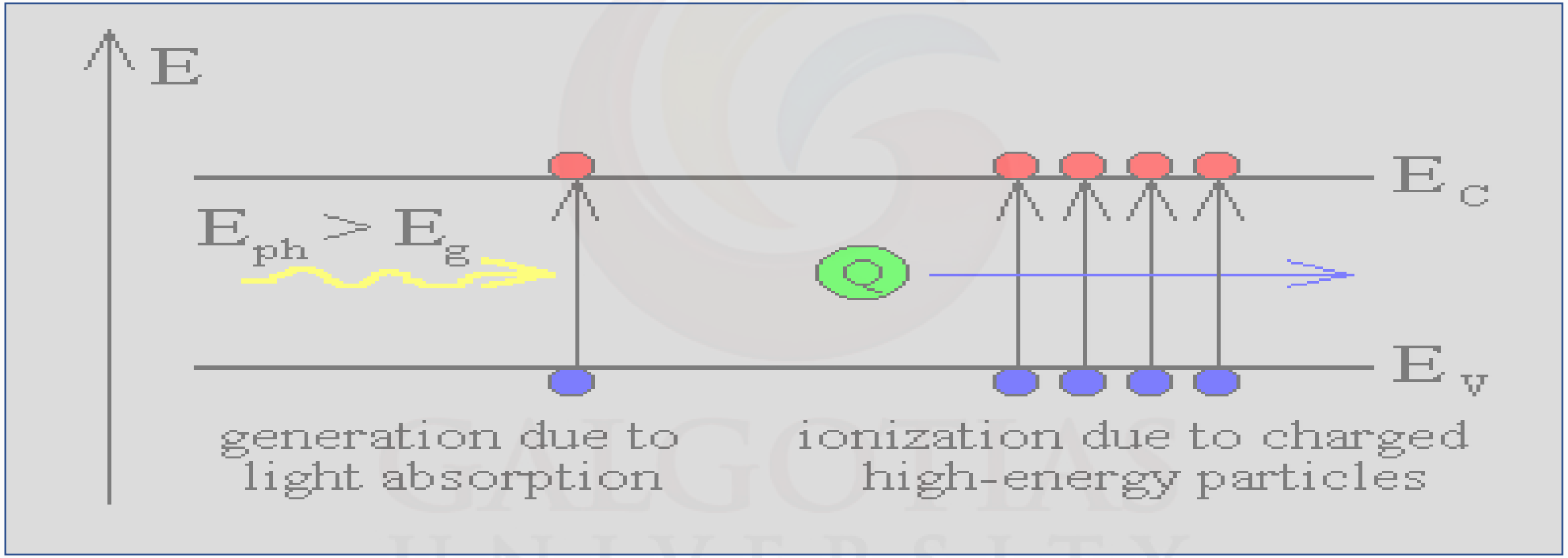
Auger recombination is a process in which an electron and a hole recombine in a band-to-band transition, but now the resulting energy is given off to another electron or hole. The involvement of a third particle affects the recombination rate so that we need to treat Auger recombination differently from band-to-band recombination.

Recombination Process

Each of these recombination mechanisms can be reversed leading to carrier generation rather than recombination. A single expression will be used to describe recombination as well as generation for each of the above mechanisms.

In addition there are **generation mechanisms** which do not have an associated recombination mechanism: generation of carriers by light absorption or a high energy electron/particle beam. These processes are also referred to as ionization processes. Impact ionization which is the generation mechanism associated with Auger recombination also belongs to this category. The generation mechanisms are illustrated with the figure below:

Recombination Process



Carrier generation due to light absorption and ionization due to high-energy particle beams

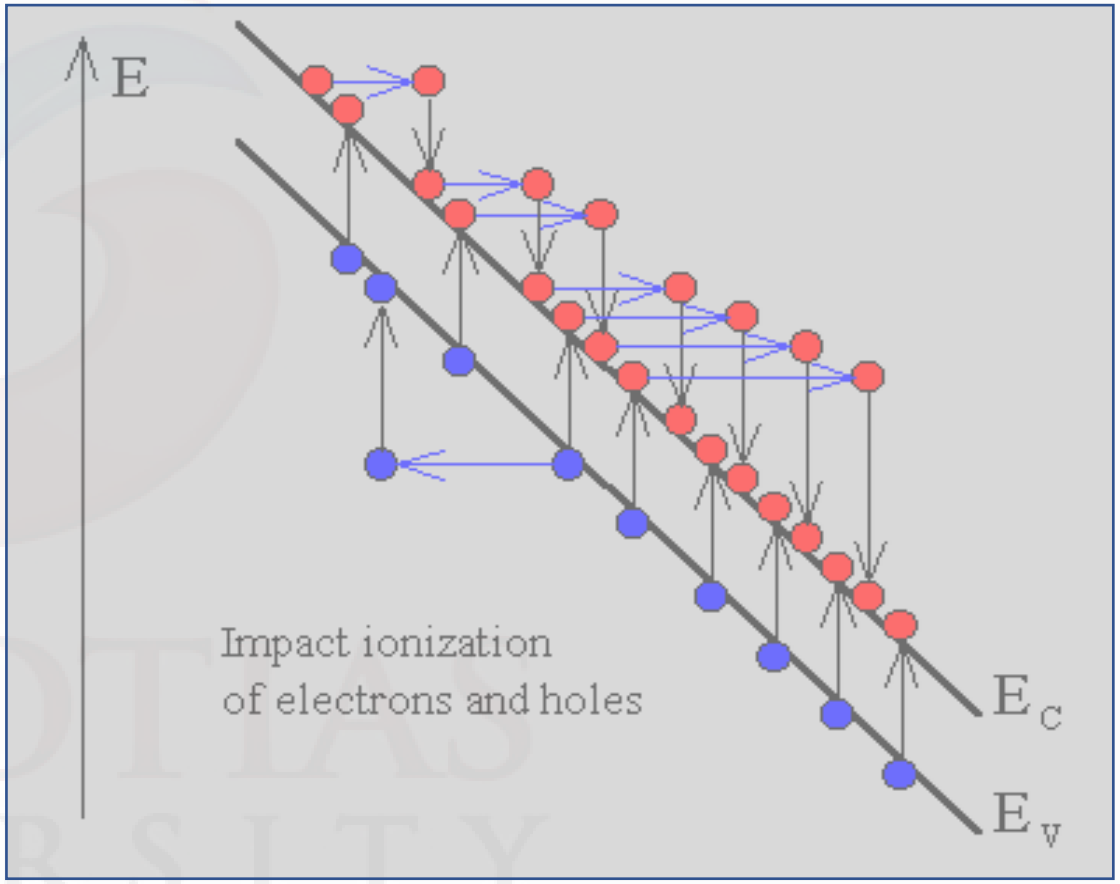
Recombination Process

Carrier **generation due to light absorption** occurs if the photon energy is large enough to lift an electron from the valence band into an empty state in the conduction band, generating one electron-hole pair. The photon energy needs to be at least equal to the bandgap energy to satisfy this condition. The photon is absorbed in this process and the excess energy, E_{ph}-E_g is added to the electron and the hole in the form of kinetic energy.

Carrier generation or **ionization due to a high energy beam** consisting of *charged* particles is similar except that the available energy can be much larger than the bandgap energy so that multiple electron-hole pairs can be formed. The high-energy particle gradually loses its energy and eventually stops. This generation mechanism is used in semiconductor-based nuclear particle counters. As the number of ionized electron-hole pairs varies with the energy of the particle, one can also use such detector to measure the particle energy.

Recombination Process

Finally there is a generation process called **impact ionization**, the generation mechanism which is the counterpart of Auger recombination. Impact ionization is caused by an electron (hole) with an energy which is much larger (smaller) than the conduction (valence) band edge. The detailed mechanism is illustrated with the figure.



Impact ionization and avalanche multiplication of electrons and holes in the presence of a large electric field.

Recombination Process

The excess energy is given off to generate an electron-hole pair through a band-to-band transition. This generation process causes avalanche multiplication in semiconductor diodes under high reverse bias: As one carrier accelerates in the electric field it gains energy. The kinetic energy is given off to an electron in the valence band, thereby creating an electron-hole pair. The resulting two electrons can create two more electrons which generate four more causing an avalanche multiplication effect. Electrons as well as holes contribute to avalanche multiplication. A simple model for the recombination-generation mechanisms states that the recombination-generation rate is proportional to the excess carrier density. It acknowledges the fact that no recombination takes place if the carrier density equals the thermal equilibrium value. The resulting expression for the recombination of electrons in a p-type semiconductor is given by:

Recombination Process

$$U_p = G_p - R_p = \frac{p_n - p_{n0}}{\tau_p}$$

and similarly for holes in an n-type semiconductor:

$$U_n = G_n - R_n = \frac{n_p - n_{p0}}{\tau_n}$$

where the parameter t can be interpreted as the average time after which an excess minority carrier recombines. We will show for each of the different recombination mechanisms that the recombination rate can be simplified to this form when applied to minority carriers in a "quasi-neutral" semiconductor. The above expressions are therefore only valid under these conditions. The recombination rates of the majority carriers equals that of the minority carriers since in steady state recombination involves an equal number of holes and electrons. As a result the recombination rate of the **majority** carriers depends on the excess **minority** carrier density which are the limiting factor in this situation.

Recombination in a depletion region and in situations where the hole and electron density are close to each other can **not** be described with the simple model and the more elaborate expressions for the individual recombination mechanisms must be used.

Carrier generation due to light absorption

Carriers can be generated in semiconductors by illuminating the semiconductor with light. The energy of the incoming photons is used to bring an electron from a lower energy level to a higher energy level. In the case where an electron is removed from the valence band and added to the conduction band, an electron-hole pair is generated. A necessary condition for this to happen is that the energy of the photon, E_{ph}, is larger than the bandgap energy, E_g. As the energy of the photon is given of to the electron, the photon no longer exists.

Assuming that each absorbed photon creates one electron-hole pair, the electron and hole generation rates are given by:

$$G_{p,light} = G_{n,light} = \alpha \frac{q P_{opt}(x)}{E_{ph} A}$$

where α is the absorption coefficient of the material at the energy of the incoming photon.

Reference:

1. J. Singh , Semiconductor optoelectronics, Physics and Technology, Mc-Graw –Hill Inc. 1995.
2. S.M. Sze, Semiconductor Devices: Physics and Technology, Wiley 2008.
3. Introduction to Nanotechnology C P Poole, Frank J. Owens, John Wiley & Sons, 2011, ISBN 978-81-265-1099-3.
4. https://ecee.colorado.edu/~bart/book/recomb.htm#generic
5. Arthur Beiser, S RaiChoudhury, ShobhitMahajan, (2009), Concepts of Modern Physics, 6th Edition, Tata-McGraw Hill. ISBN- 9780070151550.

Reference:

1. J. Singh , Semiconductor optoelectronics, Physics and Technology, Mc-Graw –Hill Inc. 1995.
2. S.M. Sze, Semiconductor Devices: Physics and Technology, Wiley 2008.
3. Introduction to Nanotechnology C P Poole, Frank J. Owens, John Wiley & Sons, 2011, ISBN 978-81-265-1099-3.
4. https://bklein.ece.gatech.edu/laser-photonics/optical-transitions-in-semiconductors/#:~:text=By%20contrast%2C%20optical%20absorption%20in,to%20the%20band%20gap%20energy.
5. Arthur Beiser, S RaiChoudhury, ShobhitMahajan, (2009), Concepts of Modern Physics, 6th Edition, Tata-McGraw Hill. ISBN- 9780070151550.

THANK YOU